106995

ground water

ENTERED

On the Use and Error of Approximation in the Domenico (1987) Solution

Michael R. West[1], Bernard H. Kueper[2], and Michael J. Ungs[3]

Abstract

A mathematical solution for solute transport in a three-dimensional porous medium with a patch source under steady-state, uniform ground water flow conditions was developed by Domenico (1987). The solution derivation strategy used an approximate approach to solve the boundary value problem, resulting in a nonexact solution. Variations of the Domenico (1987) solution are incorporated into the software programs BIOSCREEN and BIOCHLOR, which are frequently used to evaluate subsurface contaminant transport problems. This article mathematically elucidates the error in the approximation and presents simulations that compare different versions of the Domenico (1987) solution to an exact analytical solution to demonstrate the potential error inherent in the approximate expressions. Results suggest that the accuracy of the approximate solutions is highly variable and dependent on the selection of input parameters. For solute transport in a medium-grained sand aquifer, the Domenico (1987) solution underpredicts solute concentrations along the centerline of the plume by as much as 80% depending on the case of interest. Increasing the dispersivity, time, or dimensionality of the system leads to increased error. Because more accurate exact analytical solutions exist, we suggest that the Domenico (1987) solution, and its predecessor and successor approximate solutions, need not be employed as the basis for screening tools at contaminated sites.

Introduction

Analytical solutions are frequently used as screening tools to evaluate contaminant fate and transport in the subsurface environment. Analytical and semianalytical solutions are exact solutions to a boundary value problem that comprises a governing differential equation and associated boundary and initial conditions. Many approaches have been used in the published literature to derive exact analytical and semianalytical solutions (e.g., separation of variables, Laplace integral transforms, and Fourier integral transforms). Although the configuration of the domain and source zone geometry is often simplified to facilitate a tractable solution, if a correct mathematical approach is employed, the solution will be an exact analytical or semianalytical solution to the specified boundary value problem.

The governing equation for three-dimensional (3D) solute transport in saturated porous media under uniform steady-state flow subject to advection, dispersion, sorption, and first-order decay is (Bear 1979):

$$\frac{\partial C}{\partial t} + \frac{v}{R}\frac{\partial C}{\partial x} - \frac{D_x}{R}\frac{\partial^2 C}{\partial x^2} - \frac{D_y}{R}\frac{\partial^2 C}{\partial y^2} - \frac{D_z}{R}\frac{\partial^2 C}{\partial z^2} + \lambda C = 0 \quad (1)$$

where $C = C(x,y,z,t)$ is the concentration of the solute [M/L^3], y is the horizontal transverse spatial coordinate [L], z is the vertical transverse spatial coordinate [L], x is the longitudinal spatial coordinate [L], t is time [T], v is the average linear ground water velocity unidirectional in x [L/T], R is the retardation coefficient, D_x ($= \alpha_x v_x$) is

[1]Corresponding author: Department of Civil Engineering, Queen's University, Kingston, Ontario, Canada K7L 3N6; (613) 533-2130; fax (613) 533-2128; mwest@civil.queensu.ca

[2]Department of Civil Engineering, Queen's University, Kingston, Ontario, Canada K7L 3N6; (613) 533-6834; fax (613) 533-2128; kueper@civil.queensu.ca

[3]Tetra Tech Inc., 3746 Mt. Diablo Boulevard, Suite 300, Lafayette, CA 94549-3681; (510) 283-3771; fax (510) 283-0780.

Received April 2006, accepted September 2006.

Copyright © 2007 The Author(s)
Journal compilation © 2007 National Ground Water Association.

doi: 10.1111/j.1745-6584.2006.00280.x

32170

the coefficient of longitudinal dispersion [L^2/T], D_y ($= \alpha_y v_x$) is the coefficient of horizontal transverse dispersion [L^2/T], D_z ($= \alpha_z v_x$) is the coefficient of vertical transverse dispersion [L^2/T], α is the coefficient of dispersivity, and λ is the aqueous phase decay constant [1/T]. In Equation 1, both aqueous and sorbed phases undergo first-order decay. Note that the boundary value problem assumes that diffusion has a negligible contribution to transport and is ignored in the definition of D.

Several exact analytical solutions to Equation 1 have been presented in the published literature. Cleary and Ungs (1978) derived a series of exact analytic solutions, including a patch shaped source zone in a 3D domain that was semi-infinite in x and finite in y and z. The boundary value problem specified no flux boundaries at the horizontal and vertical limits of the domain, and the solution comprises two summation series. Wexler (1992) also derived an exact analytical solution to the same boundary value problem as Cleary and Ungs (1978) but considered a domain that was infinite in y and z. The solution by Wexler (1992) was an extension of an earlier exact analytical solution by Sagar (1982), who solved Equation 1 for a conservative solute. The solutions by Sagar (1982) and Wexler (1992) comprise an integral that must be numerically evaluated. Huyakorn et al. (1987), Leij et al. (1991), and Batu (1996) also derived exact analytical solutions to Equation 1 but used more sophisticated source boundary conditions than those of the foregoing authors (e.g., Gaussian distributions, multiple sources of variable concentrations). Leij et al. (1991) solve Equation 1 for the case of decay of the aqueous phase only.

An alternate approach to the aforementioned boundary value problem solutions was developed by Domenico (1987), who extended other earlier, less complex solutions proposed by Domenico and Robbins (1985) and Domenico and Palciauskas (1982). Variations of the Domenico (1987) solution were incorporated into the computer software programs BIOCHLOR (U.S. EPA 2000, 2002) and BIOSCREEN (U.S. EPA 1996), which are available to users through the U.S. EPA. These versions of the Domenico (1987) solution consider linear isothermal sorption and a variety of patch source boundary conditions. Unfortunately, a common misconception among many users of BIOCHLOR, BIOSCREEN, and other versions of the Domenico (1987) solution is that these programs use an exact analytical solution.

The Domenico (1987) solution is an approximate solution to Equation 1 and not an exact analytical solution. The solution approach used by Domenico (1987) entailed the assembly of different analytical solutions into one equation. In particular, a one-dimensional (1D) exact analytical solution for advection and longitudinal dispersion in a semiinfinite domain (e.g., Bear 1979) was used to replace the longitudinal component of a modified exact analytical solution for 3D diffusion (Crank 1975). In a preceding article (Domenico and Robbins 1985) that discussed the approach in detail, the authors identified their solution methodology as an "extended pulse approximation" and not a rigorous superposition model. The intent of the authors was to derive an approximate solution suitable for parameter estimation of field data.

The appeal of the Domenico (1987) solution is its utility. Since its derivation and resulting expression are relatively simple, modifications to boundary conditions and the governing equations (e.g., sorption or multiple species decay) are implemented with relative ease when compared to some corresponding exact analytical solutions. In addition, it can be incorporated in spreadsheet programs with little effort. Despite its frequent use, little information is available about its inherent error. Domenico and Schwartz (1998, 381) presented a limited comparison of the Domenico (1987) solution to the exact analytical solution by Leij et al. (1991) and noted "some error of approximation." It is somewhat surprising that the first investigations of error (beyond the original authors) were reported in research literature only recently (Guyonnet and Neville 2004; West and Kueper 2004; Falta et al. 2005).

It is the experience of the authors that the Domenico (1987) solution and its predecessors and successors have been adopted in some regulatory settings and readily used by the contaminant hydrogeology community as not only a screening tool but also a decision-making tool for quantifying monitored natural attenuation and carrying out risk analyses. For example, the use of BIOSCREEN and/or BIOCHLOR at contaminated sites is recommended by the U.S. EPA (1998, 2005), the United States Air Force Environmental Restoration Program (1998), and the United States Naval Facilities Engineering Command (2001). It has also been relied upon in the research literature. Huntley and Beckett (2002) and Falta et al. (2005), for example, applied the Domenico (1987) solution in various studies of plume and source zone behavior. While Falta et al. (2005) conducted a limited assessment of the inherent error for their particular work, no such effort was undertaken by Huntley and Beckett (2002).

It could be argued that the error of approximation arising from the Domenico (1987) solution is irrelevant given the uncertainties surrounding issues such as source zone delineation and aquifer heterogeneity. However, the use of the Domenico (1987) solution only exacerbates the uncertainty with approximate mathematics. The "uncertainty" due to mathematical approximation can be eliminated by choice, a luxury that cannot always be extended to complex subsurface domains. In addition, mathematical error does not fall within the definition of scientific uncertainty. Uncertainty should only be attributed to phenomena that are uncontrollable, either due to a low state in scientific knowledge or a natural complexity that is unobservable. The errors in the Domenico (1987) solution do not satisfy this definition of uncertainty. In summary, why employ an inexact mathematical model when exact versions are available?

In this paper, the approximate nature of the Domenico (1987) solution, and its predecessor and successor solutions, is investigated both mathematically and with modeling. A review of the derivations and mathematics used in these approximate solutions is first presented to elucidate errors due to solution technique, truncation, and parameter substitution. To our knowledge, such an analysis of the Domenico (1987) solution, and associated solutions, has not been published. Several simulations are then conducted to compare the output generated from the

approximate solutions to the exact analytical solutions by Cleary and Ungs (1978) and Wexler (1992). A full sensitivity analysis is not the objective of this article. Guyonnet and Neville (2004) recently conducted a thorough dimensionless comparison between the Domenico (1987) solution and an exact analytic solution by Wexler (1992) in 3D domains. It is our opinion that the use of dimensionless parameters by Guyonnet and Neville (2004) masks the errors inherent in the BIOSCREEN and BIOCHLOR models. Our approach is pragmatic, clearly illustrating the potential for error arising from the use of the Domenico (1987) solution in both two-dimensional (2D) and 3D contaminant transport applications of practical interest.

Approximations in Solution Formulation

The historical progression of the various forms of the Domenico (1987) solution and the different approximations in solution formulation are discussed in this section and highlighted in Table 1. The approximations are multiple and varied, including incorrect mathematics, truncations of exact analytic solutions, and parameter substitutions.

Throughout this section, comparisons are made between the approximate Domenico (1987) solution and other exact analytical solutions. In all cases, the comparisons reference the same boundary value problem. The objective here is to examine the impact of mathematical techniques used to derive the Domenico (1987) solution (and other related solutions), not the underlying boundary value problem assumptions or formulations.

Approximate Expression Development

The approximate technique employed by Domenico (1987) was developed earlier by Domenico and Robbins (1985), who approximated a solution for the case of advective-dispersive transport in the absence of sorption and decay. The corresponding governing equation is given by:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2}, \quad \begin{array}{r} 0 \le x \le \infty \\ -\infty \le y \le \infty \\ -\infty \le z \le \infty \end{array} \tag{2}$$

for a patch source located between $-Y/2 \le y \le Y/2$ and $-Z/2 \le z \le Z/2$, where Y is the source width and Z is the source thickness. The Domenico and Robbins (1985) technique approximates the 3D transient solution to Equation 2 using the product of 1D solutions in each direction (Domenico and Robbins 1985):

$$C(x,y,z,t) \approx C(x,t) \times C(y,t) \times C(z,t) \tag{3}$$

The methodology reflected in Equation 3 is not mathematically rigorous and introduces errors of approximation relative to exact techniques. Furthermore, Equation 3 is not a solution to the original mass transport equation and, therefore, does not conserve mass. This approach reduces to solving Equation 2 using the following three separate partial differential equations:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2}, \quad 0 \le x \le \infty \tag{4}$$

$$\frac{\partial C}{\partial t} = D_y\frac{\partial^2 C}{\partial y^2}, \quad -\infty \le y \le \infty \tag{5}$$

$$\frac{\partial C}{\partial t} = D_z\frac{\partial^2 C}{\partial z^2}, \quad -\infty \le z \le \infty \tag{6}$$

For a patch source, the exact analytic solution to Equations 5 and 6 is given by Crank (1975), which, for Equation 5 as an example, is:

$$C(y,t) = \frac{C_o}{2}\left[\operatorname{erf}\left(\frac{y + Y/2}{2\sqrt{D_y t}}\right) - \operatorname{erf}\left(\frac{y - Y/2}{2\sqrt{D_y t}}\right)\right] \tag{7}$$

where C_o is the concentration of the patch source. The exact analytical solution to Equation 4 is the Ogata and Banks (1961) solution:

$$C(x,t) = \frac{C_o}{2}\left[\operatorname{erfc}\left(\frac{x - vt}{2\sqrt{D_x t}}\right) + \exp\left(\frac{vx}{Dx}\right)\operatorname{erfc}\left(\frac{x + vt}{2\sqrt{D_x t}}\right)\right] \tag{8}$$

Table 1
Summary of Solutions

Reference	Advection (1D)	Dispersion (3D)	Decay (aqueous)	Decay (sorbed)	Sorption	$C(x,y,z,t) \approx C(x,t) \times C(y,t) \times C(z,t)$	Truncation of $C(x,t)$
Approximate expressions used in this study							
Domenico and Robbins (1985)	•	•				•	•
Domenico (1987)	•	•	•			•	•
U.S. EPA (1996)–BIOSCREEN	•	•	•		•	•	•
U.S. EPA (2000)–BIOCHLOR	•	•	•		•	•	
Guyonnet and Neville (2004)	•	•	•	•	•	•	•
Exact analytic solution used in this study							
Wexler (1992)	•	•	•	•	•		

Domenico and Robbins (1985) truncated Equation 8 in their work, thus omitting the product of the exp and erfc functions. Some discussion on the inherent error due to this truncation is found in Bear (1979) and Martin-Hayden and Robbins (1997). When Equation 3 is employed, the final truncated solution after substituting $t = x/v$ in the transverse dispersion terms is (Domenico and Robbins 1985):

$$C(x,y,z,t) \approx \frac{C_o}{8}\operatorname{erfc}\left(\frac{x-vt}{2\sqrt{D_x t}}\right) \times \left[\operatorname{erf}\left(\frac{y+Y/2}{2\sqrt{D_y\frac{x}{v}}}\right) - \operatorname{erf}\left(\frac{y-Y/2}{2\sqrt{D_y\frac{x}{v}}}\right)\right] \times \left[\operatorname{erf}\left(\frac{z+Z/2}{2\sqrt{D_z\frac{x}{v}}}\right) - \operatorname{erf}\left(\frac{z-Z/2}{2\sqrt{D_z\frac{x}{v}}}\right)\right] \tag{9}$$

The substitution of $t = x/v$ warrants some mention. Domenico and Palciauskas (1982) proposed that if time (t) is approximately equal to x/v_c, where v_c is the contaminant velocity, then the contaminant will spread from Y to $Y + (D_y t)^{1/2}$ and Z to $Z + (D_z t)^{1/2}$. While this substitution may have some conceptual utility for cases with $D_x = 0$, $D_y > 0$, and $D_z > 0$ (i.e., longitudinal plug flow), it is unclear what influence on accuracy interpreting plug flow has for cases with $D_x > 0$. The substitution was readdressed in a subsequent paper as well. Domenico and Robbins (1985) described time (t) as "running time." They continued to state that "reinterpreting this time as x/v for a moving coordinate system … has the effect of maintaining the original source dimensions at $x = 0$ so that the condition $C \cong C_o$ is maintained at $x = 0$ for $t > 0$." This interpretation of the substitution is conceptually more awkward. A rigorous mathematical solution to a boundary value problem would require no such parameter substitution to maintain the source boundary condition.

The application of Equation 3 presents another conflict that is evident in Equation 9. The product of the separate solutions for Equations 4 through 6 yields C_o^3, not C_o. This issue is not resolved by either Domenico and Robbins (1985) or Domenico (1987). However, Domenico and Schwartz (1998) provide a slightly different formulation of Equation 3 that addresses this conflict, where $C(x,y,z,t)$ is actually treated as the relative concentration $C(x,y,z,t)/C_o$, and is equal to the product of relative solutions for x, y, and z; thus, C_o^3 is replaced with C_o.

Similar to Domenico and Robbins (1985), Domenico (1987) used Equation 3 to approximate a solution for the case of advective-dispersive transport subject to aqueous phase decay in the absence of sorption. The corresponding governing equation is given by:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} - \lambda C, \quad \begin{array}{r} 0 \le x \le \infty \\ -\infty \le y \le \infty \\ -\infty \le z \le \infty \end{array} \tag{10}$$

Equation 3 was employed, which is an approach that reduces to solving Equation 10 using the following three partial differential equations:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2} - \lambda C,\ 0 \le x \le \infty \tag{11}$$

$$\frac{\partial C}{\partial t} = D_y\frac{\partial^2 C}{\partial y^2},\ -\infty \le y \le \infty \tag{12}$$

$$\frac{\partial C}{\partial t} = D_z\frac{\partial^2 C}{\partial z^2},\ -\infty \le z \le \infty \tag{13}$$

Again, the exact analytical solution to Equations 12 and 13 is given by Crank (1975) as presented in Equation 7. The exact analytical solution to Equation 11 is given by Bear (1979):

$$C(x,t) = \frac{C_o}{2}\left\{\exp\left\{\frac{xv}{2D_x}\left[1 - \sqrt{1 + \frac{4\lambda D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x - vt\sqrt{1 + \frac{4\lambda D_x}{v^2}}}{2\sqrt{D_x t}}\right) + \exp\left\{\frac{xv}{2D_x}\left[1 + \sqrt{1 + \frac{4\lambda D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x + vt\sqrt{1 + \frac{4\lambda D_x}{v^2}}}{2\sqrt{D_x t}}\right)\right\} \tag{14}$$

where Equation 14 is the nontruncated (full) 1D analytic solution to Equation 11. Both the truncated and nontruncated solutions are presented in Bear (1979), where the truncated solution omits the second product of exp and erfc. Domenico (1987) employed the truncated solution. Using Equation 3 and the substitution $t = x/v_c$ (with $v_c = v$), the completed Domenico (1987) solution is:

$$C(x,y,z,t) \approx \frac{C_o}{8}\exp\left\{\frac{xv}{2D_x}\left[1 - \sqrt{1 + \frac{4\lambda D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x - vt\sqrt{1 + \frac{4\lambda D_x}{v^2}}}{2\sqrt{D_x t}}\right) \times \left[\operatorname{erf}\left(\frac{y + Y/2}{2\sqrt{D_y\frac{x}{v}}}\right) - \operatorname{erf}\left(\frac{y - Y/2}{2\sqrt{D_y\frac{x}{v}}}\right)\right] \times \left[\operatorname{erf}\left(\frac{z + Z/2}{2\sqrt{D_z\frac{x}{v}}}\right) - \operatorname{erf}\left(\frac{z - Z/2}{2\sqrt{D_z\frac{x}{v}}}\right)\right] \tag{15}$$

An interesting issue arises in Equation 15 with the substitution of $t = x/v_c$. Since v_c is the contaminant velocity for this substitution, one can rationalize $v_c = v/R$ (for $D_x = 0$), but the treatment of decay (λ) is more awkward. Decay in the transverse direction has been excluded in all derivations to date and thus introduces an additional error of approximation to Domenico (1987) type solutions that incorporate decay. Furthermore, the application of Equation 3 reduces the 3D decay stated in Equation 10 to 1D decay in only the x direction (e.g., Bear 1979).

Adoption of Domenico and Robbins (1985) and Domenico (1987) in subsequent studies

The Domenico and Robbins (1985) technique of employing Equation 3 was implemented in BIOCHLOR (U.S. EPA 2000, 2002), BIOSCREEN (U.S. EPA 1996), and Guyonnet and Neville (2004) to approximate 1D advection with 3D dispersion, including linear isothermal sorption and first-order decay (see Table 1); both Equation 3 and the truncation of Equations 8 and 14 were implemented in the latter two solutions. The original Domenico and Robbins (1985) and Domenico (1987) solutions differ from those in BIOSCREEN, BIOCHLOR, and Guyonnet and Neville (2004) in that the latter solutions incorporate sorption. BIOCHLOR and BIOSCREEN consider decay in only the aqueous phase, while Guyonnet and Neville (2004) examine decay in both the aqueous and sorbed phases.

The governing equation describing advection, dispersion, linear isothermal sorption, and first-order decay in both the aqueous and sorbed phases is given by Equation 1. If Equation 3 is employed, Equation 1 is reduced to the following three partial differential equations that must be solved individually:

$$\frac{\partial C}{\partial t} = -\frac{v}{R}\frac{\partial C}{\partial x} + \frac{D_x}{R}\frac{\partial^2 C}{\partial x^2} - \lambda C,\ 0 \le x \le \infty \tag{16}$$

$$\frac{\partial C}{\partial t} = \frac{D_y}{R}\frac{\partial^2 C}{\partial y^2},\ -\infty \le y \le \infty \tag{17}$$

$$\frac{\partial C}{\partial t} = \frac{D_z}{R}\frac{\partial^2 C}{\partial z^2},\ -\infty \le z \le \infty \tag{18}$$

The exact analytical solution to Equation 16 is given by Bear (1979):

$$C(x,t) = \frac{C_o}{2}\left\{\exp\left\{\frac{xv}{2D_x}\left[1 - \sqrt{1 + \frac{4\lambda R D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x - \frac{vt}{R}\sqrt{1 + \frac{4\lambda R D_x}{v^2}}}{2\sqrt{\frac{D_x}{R}t}}\right) + \exp\left\{\frac{xv}{2D_x}\left[1 + \sqrt{1 + \frac{4\lambda R D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x + \frac{vt}{R}\sqrt{1 + \frac{4\lambda R D_x}{v^2}}}{2\sqrt{\frac{D_x}{R}t}}\right)\right\} \tag{19}$$

The solutions to Equations 17 and 18 can be derived using the techniques described by Crank (1975), resulting in:

$$C(y,t) = \frac{C_o}{2}\left[\operatorname{erf}\left(\frac{y + Y/2}{2\sqrt{\frac{D_y}{R}t}}\right) - \operatorname{erf}\left(\frac{y - Y/2}{2\sqrt{\frac{D_y}{R}t}}\right)\right] \tag{20}$$

$$C(z,t) = \frac{C_o}{2}\left[\operatorname{erf}\left(\frac{z + Z/2}{2\sqrt{\frac{D_z}{R}t}}\right) - \operatorname{erf}\left(\frac{z - Z/2}{2\sqrt{\frac{D_z}{R}t}}\right)\right] \tag{21}$$

Employing Equation 3 yields the final approximate nontruncated solution:

$$C(x,y,z,t) = \frac{C_o}{8}\left\{\exp\left\{\frac{xv}{2D_x}\left[1 - \sqrt{1 + \frac{4\lambda R D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x - \frac{vt}{R}\sqrt{1 + \frac{4\lambda R D_x}{v^2}}}{2\sqrt{\frac{D_x}{R}t}}\right) + \exp\left\{\frac{xv}{2D_x}\left[1 + \sqrt{1 + \frac{4\lambda R D_x}{v^2}}\right]\right\} \times \operatorname{erfc}\left(\frac{x + \frac{vt}{R}\sqrt{1 + \frac{4\lambda R D_x}{v^2}}}{2\sqrt{\frac{D_x}{R}t}}\right)\right\} \times \left[\operatorname{erf}\left(\frac{y + Y/2}{2\sqrt{\frac{D_y}{R}t}}\right) - \operatorname{erf}\left(\frac{y - Y/2}{2\sqrt{\frac{D_y}{R}t}}\right)\right] \times \left[\operatorname{erf}\left(\frac{z + Z/2}{2\sqrt{\frac{D_z}{R}t}}\right) - \operatorname{erf}\left(\frac{z - Z/2}{2\sqrt{\frac{D_z}{R}t}}\right)\right] \tag{22}$$

Equation 22 is the nontruncated form of the approximate solution to Equation 1 using the Domenico and Robbins (1985) technique (i.e., Equation 3). If the substitution of $t = x/v_c$ (with $v_c = v/R$) is made in the erf terms, Equation 22 becomes the solution used in BIOCHLOR.

The exact analytical solution to Equation 1 was originally derived by Cleary and Ungs (1978) for a finite transverse domain. By considering an infinite transverse domain, Sagar (1982) derived an exact solution to Equation 1 for the case of a conservative solute. Based on the work by Sagar (1982), Wexler (1992) derived an exact analytical solution to Equation 1. The exact solution presented by Wexler (1992) can be used to further illustrate

error in the Domenico (1987) solution and the approach by Domenico and Robbins (1985). The exact analytical solution to Equation 1 presented by Wexler (1992) is:

$$C(x,y,z,t) = C_o\frac{x}{8}\sqrt{\frac{R}{\pi D_x}}\exp\left[\frac{xv}{2D_x}\right]\int_0^t \tau^{-3/2} \times \exp\left\{-\left(\lambda + \frac{v^2}{4D_xR}\right)\tau - \frac{x^2R}{4D_x\tau}\right\} \times \left\{\mathrm{erf}\left[\left(y+\frac{Y}{2}\right)\sqrt{\frac{R}{4D_y\tau}}\right] - \mathrm{erf}\left[\left(y-\frac{Y}{2}\right)\sqrt{\frac{R}{4D_y\tau}}\right]\right\} \times \left\{\mathrm{erf}\left[\left(z+\frac{Z}{2}\right)\sqrt{\frac{R}{4D_z\tau}}\right] - \mathrm{erf}\left[\left(z-\frac{Z}{2}\right)\sqrt{\frac{R}{4D_z\tau}}\right]\right\}\mathrm{d}\tau \tag{23}$$

where τ is the dummy variable of integration. The Domenico and Robbins (1985) technique (i.e., Equation 3) essentially removes the transverse error functions (erf) from the integration and treats the τ as a constant t, giving:

$$C(x,y,z,t) = C_o\frac{x}{8}\sqrt{\frac{R}{\pi D_x}}\exp\left[\frac{xv}{2D_x}\right]\int_0^t \tau^{-3/2} \times \exp\left\{-\left(\lambda + \frac{v^2}{4D_xR}\right)\tau - \frac{x^2R}{4D_x\tau}\right\}\mathrm{d}\tau \times \left\{\mathrm{erf}\left[\left(y+\frac{Y}{2}\right)\sqrt{\frac{R}{4D_yt}}\right] - \mathrm{erf}\left[\left(y-\frac{Y}{2}\right)\sqrt{\frac{R}{4D_yt}}\right]\right\} \times \left\{\mathrm{erf}\left[\left(z+\frac{Z}{2}\right)\sqrt{\frac{R}{4D_zt}}\right] - \mathrm{erf}\left[\left(z-\frac{Z}{2}\right)\sqrt{\frac{R}{4D_zt}}\right]\right\} \tag{24}$$

The x component of Equation 24 is actually the solution by Bear (1979) presented in Equation 19; hence, once the integral is analytically evaluated, Equation 24 reduces to Equation 22. There is no mathematical basis to justify Equation 3 or the approximation of $\tau = t$ in Equation 24; it is a matter of convenience.

Based on the aforementioned approximations, it is anticipated that source width, source depth, transverse dispersion, retardation, transverse dimensionality, and time (or the substitution of $t = x/v_c$) will contribute to the "error of approximation." In some instances, the conditions where the error is minimized can be surmised from the properties of the error function (erf). The erf is an asymptotic exponential integral where erf(∞) $\rightarrow$ 1. Therefore, large values of the argument (i.e., the ratio of the numerator to the denominator) will yield error function values close to 1, and the transverse components of Equation 24 can become negligible. In relative terms, large source geometries (Y and Z), large values of R, large values of v_c, small values of D_y and D_z, and small values of x should reduce the influence of the transverse components when examining concentrations along the plume centerline ($y = z = 0$). Thus, under these conditions, a Domenico (1987) type solution approaches the exact 1D analytical solution of Bear (1979) presented in Equation 19. As a consequence, a practitioner conducting a suite of screening calculations with a Domenico (1987) type solution will encounter increasing or decreasing errors of approximation depending on the choice of parameter.

Quantification of the Error of Approximation

The relative error (σ) is evaluated using:

$$\sigma(\%) = \frac{(O_D - O_W)}{O_W} \times 100 \tag{25}$$

where O_D is the output from the approximate Domenico (1987) solution, and O_W is the output from the exact analytical solutions by Cleary and Ungs (1978) and Wexler (1992); For all cases, the solutions by Cleary and Ungs (1978) and Wexler (1992) produced the same results. For convenience, reference will be made to only Wexler (1992) hereafter. The solution by Wexler (1992) (Equation 23) requires numerical integration techniques to evaluate the integral. This need for numerical integration prevents analytical analysis of the relative error between the exact analytical solution by Wexler (1992) and the approximate solutions presented by Domenico and Robbins (1987), Domenico (1987), U.S. EPA (1996, 2000, 2002), and Guyonnet and Neville (2004). Thus, a comparative evaluation, as presented Equation 25, is necessary.

Comparison of Solutions and Input Parameters

Simulations are executed here for both 2D and 3D porous media with a constant concentration patch source by comparing Domenico (1987) to Wexler (1992) for both transient and steady-state conditions. Exact analytical solutions by Huyakorn et al. (1987), Leij et al. (1991), and Batu (1996) could also have been used for this purpose. The 3D cases simulate an aquifer with only a partially penetrating source zone, while the 2D case considers a source zone distributed through the full aquifer thickness. The consideration of dimensionality not only highlights the influence of domain configuration on the error of approximation in Domenico (1987) but also illustrates the differences in prediction for the two cases, which can be overlooked while screening a site. We assume that our example site is fairly well characterized, such that field solute concentrations, hydraulic gradient, and geological conditions are known. We assume that the contaminant is trichloroethene with a source concentration (C_o) of 11 mg/L, and all concentration values are assessed along the plume centerline, $C(x,0,0,t)$, for all simulations. In addition, the plume length (L_p), defined by the position of the 5 parts per billion contour, is assumed to be 100 m for the purposes of calculating a constant

dispersivity. The parameters are summarized in Table 2. Note that $R = 1$ for all simulations as the Domenico (1987) solution does not incorporate sorption. The depth of the source zone below the water table is 2.5 m.

One would normally conduct a suite of screening simulations to investigate the influence of various parameters (e.g., velocity, source width) on the solution output. A subset of simulations is conducted herein, where only the dispersivity values are adjusted. A full dimensionless analysis was conducted by Guyonnet and Neville (2004). As mentioned in the previous section, transverse dispersion and dimensionality will potentially introduce significant error due to the mathematical approximations employed in the Domenico and Robbins (1985) technique. The three approaches suggested in the BIOCHLOR manual (U.S. EPA 2000, 2002) are implemented to obtain reasonable dispersivities for the subject example site. In the first approach, the longitudinal dispersivity (α_x) is 10% of the L_p; using this approach, a constant $\alpha_x =$ 10 m is calculated for all values of x. The second and third approaches recognize the scale dependent nature of dispersivity (Gelhar et al. 1992). The method of Pickens and Grisak (1981) is adopted where $\alpha_x = 0.1\ L$, where L is the distance along the domain to the point of reference. The third method uses the findings of Xu and Eckstein (1995) where $\alpha_x = 0.83(\log_{10}L)^{2.414}$; in the latter two approaches, α_x increases with x (i.e., L). For this example, the horizontal transverse dispersivity is given by $\alpha_y = 0.1\alpha_x$ and, where appropriate, the vertical transverse dispersivity is given by $\alpha_z = 0.01\alpha_x$. Both transient and steady-state simulations were executed in the 2D study by assuming that the vertical transverse dispersivity was negligible (i.e., $\alpha_z = 0$ and $D_z = 0$). Descriptions of the steady-state and transient simulations are provided in Tables 3 and 4, respectively. The relative error between solution outputs for each of the simulations is evaluated using Equation 25.

Finally, a series of transient 3D simulations are conducted to demonstrate the error due to truncation of the solution for $C(x,t)$. These simulations are summarized in Table 5 and use the parameters listed in Table 2 where appropriate. Relative error is evaluated along the plume centerline while employing dispersivity values calculated using $\alpha_x = 0.1\ L$.

Table 2
Summary of Input Parameters for All Simulations

Description	Parameter	Value
Source concentration	C_o	11 mg/L
Source width	Y	10 m
Source depth below the water table (3D case)	$Z/2$	2.5 m
Source depth below the water table (2D case)	$Z/2$	2.5 m
Source decay half-life	$t(\gamma)_{1/2}$	∞
Solute plume decay half-life	$t(\lambda)_{1/2}$	5 years
Hydraulic gradient	∇h	0.008
Hydraulic conductivity	K	1×10^{-4} m/s
Longitudinal dispersivity	α_x	Various
Transverse horizontal dispersivity	α_y	$0.1\alpha_x$
Transverse vertical dispersivity	α_z	$0.01\alpha_x$
Porosity	θ	0.25
Ground water velocity	v	0.277 m/d
Solute retardation factor	R	1.0

Table 3
Summary of Steady-State Simulations

Run	Solution	Configuration	α_x
1	Wexler (1992)	2D	10 m
2	Domenico (1987)	2D	10 m
3	Wexler (1992)	2D	0.1 L
4	Domenico (1987)	2D	0.1 L
5	Wexler (1992)	3D	10 m
6	Domenico (1987)	2D	10 m
7	Wexler (1992)	3D	0.1 L
8	Domenico (1987)	3D	0.1 L

Steady-State Simulations

Steady-state concentration profiles for solute transport in 2D and 3D porous media are presented in Figure 1, which compares the output generated from solutions by Domenico (1987) and Wexler (1992). The simulations are conducted using either a constant $\alpha_x = 10$ m or a variable $\alpha_x = 0.1\ L$. Clearly, the solutions are sensitive to the choice of dispersivity, with the variable α_x producing greater concentrations near the source zone and reduced concentrations downstream relative to the constant α_x. Furthermore, the dimensionality of the problem has a significant impact on the concentration profiles, which underscores the need for dimensional screening at sites.

The relative error between the two solutions is presented in Figure 2 for the four combinations of dispersivity and dimension. The Domenico (1987) solution

Table 4
Summary of Transient Simulations

Run	Case	Solution	Distance to Monitoring Well (m)	Method of Calculating α_x
1	A	Wexler (1992)	10	Xu and Eckstein (1995)
2	A	Domenico (1987)	10	Xu and Eckstein (1995)
3	A	Wexler (1992)	100	Xu and Eckstein (1995)
4	A	Domenico (1987)	100	Xu and Eckstein (1995)
5	B	Wexler (1992)	10	Pickens and Grisak (1981)
6	B	Domenico (1987)	10	Pickens and Grisak (1981)
7	B	Wexler (1992)	100	Pickens and Grisak (1981)
8	B	Domenico (1987)	100	Pickens and Grisak (1981)

Table 5
Simulation Notation for Figure 5

Label	Description
Full 1 year	Relative error between Wexler (1992) and the full (nontruncated) Domenico (1987) solution (e.g., BIOCHLOR) for 1 year
Truncated 1 year	Relative error between Wexler (1992) and the truncated Domenico (1987) solution (i.e., Domenico [1987] and BIOSCREEN) for 1 year
Full 2 years	Relative error between Wexler (1992) and the full (nontruncated) Domenico (1987) solution (e.g., BIOCHLOR) for 2 years
Truncated 2 years	Relative error between Wexler (1992) and the truncated Domenico (1987) solution (i.e., Domenico [1987] and BIOSCREEN) for 2 years
Full 5 years	Relative error between Wexler (1992) and the full (nontruncated) Domenico (1987) solution (e.g., BIOCHLOR) for 5 years
Truncated 5 years	Relative error between Wexler (1992) and the truncated Domenico (1987) solution (i.e., Domenico [1987] and BIOSCREEN) for 5 years

underpredicts the steady-state concentrations through the majority of the domain, with the exception of the constant α_x for distances close to the source zone. As suggested earlier from mathematical considerations, the error in the Domenico (1987) solution is exacerbated by increasing the dimensionality of the domain from 2D to 3D. The choice of either a constant or variable α_x has a significant impact on the behavior of the error. For the 3D case, the constant α_x produces relative errors ranging from 2.5% to −24%, peaking near the source zone. However, the

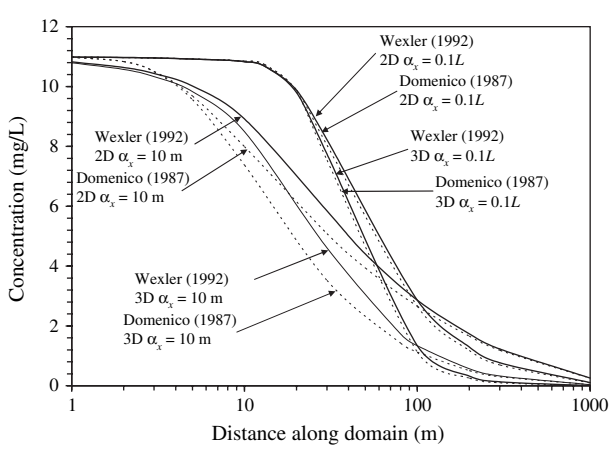

Figure 1. Comparison of solutions for steady-state conditions in 2D and 3D porous media. Simulations are summarized in Table 3.

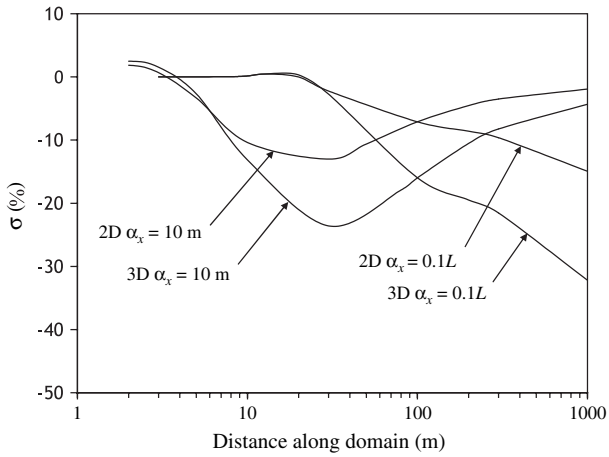

Figure 2. Relative error between Wexler (1992) and Domenico (1987) for 2D and 3D steady-state simulations.

variable α_x yields an error of 0.5% near the source zone that continually increases with distance, such that an error of −32% is realized at a distance of approximately 1000 m.

Transient Simulations

Breakthough curves are presented in Figure 3 for monitoring wells located at 10 and 100 m downstream of the source. Case A uses dispersivities calculated from Xu and Eckstein (1995), while the method of Pickens and Grisak (1981) is used in case B. The case A α_x values for the 10- and 100-m wells are 0.83 and 4.42 m, respectively. The α_x values of 1 and 10 m were applied to the 10- and 100-m wells for case B, respectively.

Figure 3 illustrates that the Domenico (1987) solution can underpredict the concentrations at each well for all times. The relative error associated with the underprediction is presented in Figure 4. The error between Wexler (1992) and Domenico (1987) is significant at early time for all wells, with values of −30% for the 10-m well and −80% for the 100-m well. For late time, the well near the source zone (10 m) exhibits negligible error. However, the error at the 100 m well achieves a steady-state relative error of −7% for case A but −16% for case B. It can be observed that increasing the dispersion in the system increases the error between the solutions.

Influence of Truncation in $C(x,t)$

Profile curves of relative error between the truncated and nontruncated Domenico (1987) solutions (see Table 5) and Wexler (1992) are presented in Figure 5. A total of six simulations were conducted to examine the relative error at $t = 1$, 2, or 5 years for Equation 25.

The influence of truncating $C(x,t)$ can be observed by comparing the relative error calculations for each simulation. The truncated cases (e.g., Domenico [1987] and BIOSCREEN) yield additional error of approximation when compared to the nontruncated cases (e.g., BIOCHLOR); however, all cases produce significant error with increasing x. At a time of 1 year and a distance of 100 m, the

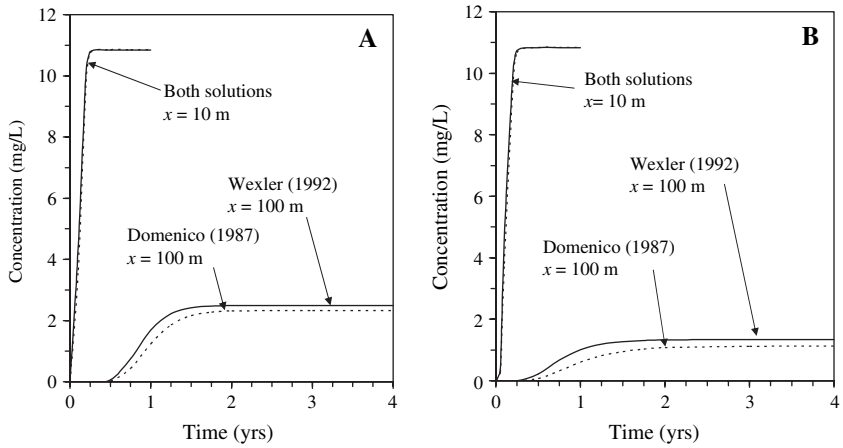

Figure 3. Comparison of breakthrough curves at x = 10 and 100 m between Wexler (1992) and Domenico (1987). (Case A) Simulations with dispersivities calculated using Xu and Eckstein (1995). (Case B) Dispersivities calculated using Pickens and Grisak (1981). Simulations are summarized in Table 4.

nontruncated Domenico (1987) solution produced a relative error of −32%, but the truncated Domenico (1987) solution yields a relative error of −41%. The additional error of approximation diminishes with increasing time as the two solutions approach steady-state conditions.

Conclusions

The accuracy of the Domenico (1987) solution is parameter dependent. Depending on the choice of parameters, the magnitude of relative error can range from significant (e.g., −80%) to negligible. When comparing Domenico (1987) to the exact analytical solutions of Cleary and Ungs (1978) and Wexler (1992), the Domenico (1987) solution typically underpredicts concentrations. The magnitude of relative error is a function of parameter value, time, and dimensionality; the application of dispersivity is particularly awkward as different techniques yield variable error behavior. Most important, the behavior and magnitude of the relative error cannot be predicted a priori. Thus, users of the Domenico (1987) solution and other associated versions cannot ascertain the degree of underprediction without a comparative study (as conducted herein) or potentially by examining the type curves of Guyonnet and Neville (2004).

Additional relative error is observed in expressions (i.e., BIOSCREEN and Domenico [1987]) that truncate the analytical solution for 1D solute transport. When performing simulations to evaluate the effects of solution formulation and truncation, the relative error between the exact analytical solutions by Cleary and Ungs (1978) and Wexler (1992) and the various approximate expressions (i.e., Domenico [1987]; BIOSCREEN; BIOCHLOR) ranged from 2% to −80%, depending on the case of interest.

Guyonnet and Neville (2004) stated that along the plume centerline, and for ground water flow regimes dominated by advection and mechanical dispersion rather than by molecular diffusion, the discrepancies between

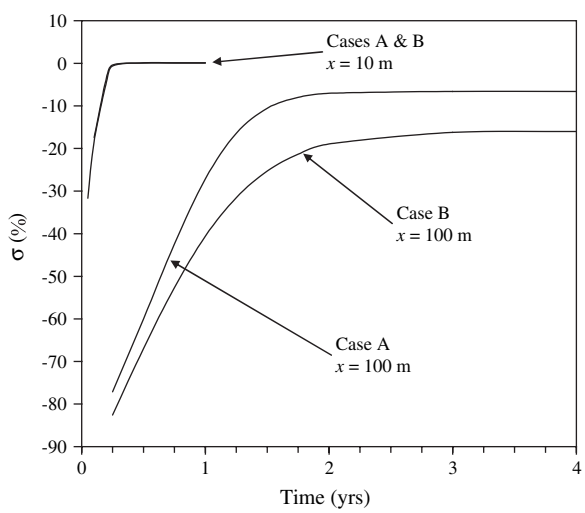

Figure 4. Relative error for breakthrough curves at x = 10 and 100 m between Wexler (1992) and Domenico (1987). Case A denotes simulations with dispersivities calculated using Xu and Eckstein (1995) while dispersivities calculated using Pickens and Grisak (1981) are presented in case B.

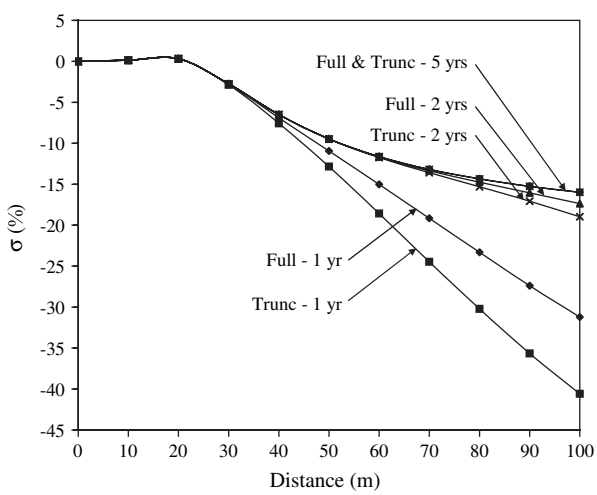

Figure 5. Transient 3D comparison of relative error between different approximate expressions and Wexler (1992) at t = 1, 2, and 5 years. Longitudinal dispersivity was estimated using α_x = 0.1 L. Refer to Table 5 for label descriptions.

the Domenico (1987) solution and the exact Sagar (1982) solution can be considered negligible for practical purposes. Based on Figures 1 through 5 of this work, we take a more conservative stance and suggest that in the context of maximum allowable concentrations at contaminated sites, the solutions developed using the technique by Domenico and Robbins (1985) can potentially significantly underpredict solute concentrations along the plume centerline when compared to other exact analytical solutions for both transient and steady-state conditions in 2D and 3D domains.

Given the aforementioned magnitude of relative error and the abundance of exact analytical solutions available to practitioners, the Domenico (1987) solution and its associated solutions need not be employed as screening tools. We fully encourage practitioners to use peer-reviewed published exact analytic solutions, preferably with open source code. In some cases, a compiled program with a graphic user interface is more desirable. There are many such software packages available in industry. While not a comprehensive list, some examples of commercial software that use exact analytical solutions include PRINCE (distributed by Waterloo Hydrogeologic Inc.), ATRANS (S.S. Papadopulos Inc.), and SOLUTRANS (Fitts Geosolutions).

Acknowledgments

Funding for this work was provided by Texas Instruments Inc. Additional funding was provided by the Ontario Graduate Scholarship Program, the Natural Sciences and Engineering Research Council of Canada, and Queen's University in the form of student scholarships to the senior author. The authors would also like to acknowledge and thank the four anonymous reviewers for their thorough and insightful comments.

References

Batu, V. 1996. A generalized three-dimensional analytical solute transport model for multiple rectangular first-type sources. *Journal of Hydrology* 174, 57–82.

Bear, J. 1979. *Hydraulics of Ground Water*. New York: McGraw-Hill.

Cleary, R., and M. Ungs. 1978. Report No. 78-WR-15, Water Resources Program. Princeton, New Jersey: Princeton University.

Crank, J. 1975. *The Mathematics of Diffusion*. New York: Oxford University Press.

Domenico, P.A. 1987. An analytical model for multidimensional transport of a decaying contaminant species. *Journal of Hydrology* 91, 49–58.

Domenico, P.A., and F.W. Schwartz. 1998. *Physical and Chemical Hydrology*, 2nd ed. New York: John Wiley & Sons Inc.

Domenico, P.A., and G.A. Robbins. 1985. A new method of contaminant plume analysis. *Ground Water* 23, no. 4: 476–485.

Domenico, P.A., and V.V. Palciauskas. 1982. Alterative boundaries in solid waste management. *Ground Water* 20, no. 3: 303–311.

Falta, R., N. Basu, and R. Rao. 2005. Assessing impacts of partial mass depletion in DNAPL source zones: II. Coupling source strength functions to plume evolution. *Journal of Contaminant Hydrology* 79, 45–66.

Guyonnet, D., and C. Neville. 2004. Dimensionless analysis of two analytical solutions for 3-D solute transport in groundwater. *Journal of Contaminant Hydrology* 75, 141–153.

Huntley, D., and G. Beckett. 2002. Persistence of LNAPL sources: Relationship between risk reduction and LNAPL recovery. *Journal of Contaminant Hydrology* 59, 3–26.

Huyakorn, P., M. Ungs, L. Mulkey, and E. Sudicky. 1987. A three-dimensional analytical method for predicting leachate migration. *Ground Water* 25, no. 5: 588–598.

Leij, F., T. Skaggs, and M. van Genuchten. 1991. Analytical solutions for solute transport in three-dimensional semi-infinite porous media. *Water Resources Research* 27, no. 10: 2719–2733.

Martin-Hayden, J., and G. Robbins. 1997. Plume distortion and apparent attenuation due to concentration averaging in monitoring wells. *Ground Water* 35, no. 2: 339–346.

Ogata, A., and R. Banks. 1961. A solution of the differential equation of longitudinal dispersion in porous media. USGS Prof. Pap. No. 411-A. Reston, Virginia: USGS.

Pickens, J., and G. Grisak. 1981. Scale-dependent dispersion in a stratified granular aquifer. *Water Resources Research* 17, no. 4: 1191–1211.

Sagar, B. 1982. Dispersion in three dimensions: Approximate analytical solutions. *ASCE, Journal of Hydraulics Division* 108, no. HY1: 47–62.

United States Air Force Environmental Restoration Program. 1998. *Handbook for Remediation of Petroleum-Contaminated Sites (A Risk Based Strategy)*. Prepared for Air Force Center for Environmental Excellence, Technology Transfer Division.

United States Naval Facilities Engineering Command. 2001. Guidance for Optimizing Remedial Action Operation (RAO), Special Report SR-2101-ENV. Prepared for Department of the Navy RAO/LTM Optimization Working Group.

U.S. EPA. 2005. Monitored Natural Attenuation of MTBE as a Risk Management Option at Leaking Underground Storage Tank Sites, EPA/600/R-04/1790. Washington, DC: U.S. EPA, Office of Research and Development.

U.S. EPA. 2002. BIOCHLOR Natural Attenuation Decision Support System. Version 2.2 User's Manual Addendum. Washington, DC: U.S. EPA.

U.S. EPA. 2000. BIOCHLOR Natural Attenuation Decision Support System. User's Manual Version 1.0, EPA/600/R-00/008. Washington, DC: US EPA, Office of Research and Development.

U.S. EPA. 1998. Technical Protocol for Evaluating Natural Attenuation of Chlorinated Solvents in Ground Water, EPA/600/R-98/128. Washington, DC: US EPA, Office of Research and Development.

U.S. EPA. 1996. BIOSCREEN—Natural Attenuation Decision Support System. User's Manual Version 1.3, EPA/600/R-96/087. Washington, DC: National Risk Management Research Laboratory, Office of Research and Development.

West, M., and B. Kueper. 2004. Natural attenuation of solute plumes in bedded fractured rock. In *Proceedings of the U.S. EPA/NGWA Fractured Rock Conference: State of Science and Measuring Success in Remediation*. National Ground Water Association, NGWA Press.

Wexler, E. 1992. Analytical solutions for one-, two-, and three-dimensional solute transport in groundwater systems with uniform flow. In *Techniques of Water Resources Investigations of the United States Geological Survey, chap. B7, Book 3, Applications of Hydraulics*, 53–55.

Xu, M., and Y. Eckstein. 1995. Use of weighted least-squares method in evaluation of the relationship between dispersivity and field scale. *Ground Water* 33, no. 6: 905–908.